

REMARKS

Claims 1, 5, 9, and 13-27 are pending in the above-identified application, the remaining claims having been withdrawn from consideration. Claims 1, 5, 9, and 13-27 stand rejected under 35 U.S.C. § 103(a). Applicant traverses all rejections and respectfully requests reconsideration of the claims in light of the amendments and remarks made in this response.

Applicant's Invention

The invention is directed to a method for use in deriving a chemical structure diagram. The method includes identifying, from a connection table for a chemical structure, an instance of structural symmetry in the chemical structure and positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry.

Amendments

With this Response, claims 1, 5, and 9 have been amended to more particularly point out the invention. No new matter has been added by this amendment. Support for this amendment is found throughout the specification, for example at page 6, line 18 through page 7, line 2 and page 7, lines 16-17; and page 9, lines 1-15.

Also with the Response, the title of the application has been amended as shown above.

Finally, with this submission, Applicant has also submitted a Request for Change of Attorney Docket Numbers. The new docket number is 103544.131 US2. The previous docket number was 103544.127.

Objection to the Specification

The Office Action objects to the specification as having an allegedly deficient background section. Specifically, the Office Action states "Applicants have not indicated any problems in the prior art which they are attempting to solve." The Office Action also suggests

that the background section does not comment on alleged prior art, such as connection tables and chemical symmetry. Applicant objects to the objection as improper.

The sections in the MPEP regarding the arrangement of the application and its contents are guidelines; they are not mandatory. The only requirement of the specification is that it “must be in such full, clear, concise, and exact terms as to enable any person skilled in that art or science to which the invention pertains to make and use the same.” 37 C.F.R. § 1.71; MPEP § 608.01. The background section is not a required section for all patent applications. The arrangement of the application is defined in 37 C.F.R. § 1.77, which states, “The elements of the application, if applicable, should appear in the following order...” (emphasis added). Similarly, MPEP § 608.01(a) states, “the order of arrangement of specification elements is preferable...” (emphasis added). Regarding the content of the background section, the MPEP merely states, “Where applicable, the problems involved in the prior art or other information disclosed which are solved by the applicant’s invention should be indicated.” MPEP § 608.01(c). Thus, Applicant respectfully asserts that a statement regarding a problem to be solved by his invention is not required.

Nevertheless, Applicant has amended the specification to add two paragraphs at page 4. These paragraphs are located in the “Detailed Description” section of the application. Applicant submits this is an appropriate location for the amended information as it flows logically from the previous paragraph discussing structural diagram generation.

In addition, Applicant brings to the Examiner’s attention the submission dated April 9, 2004, responding to the Examiner’s request for information under 37 C.F.R. § 1.105. Starting at page 4 of that submission, Applicant explains some of the improvements of the present invention over some of Applicant’s (or Assignee’s) earlier commercial products. Specifically, Applicant

stated that earlier commercial products did not consult symmetry or other features encompassed by the instant invention when creating two-dimensional chemical structures. In addition, Applicant stated that other packages attempting to provide this ability “differed from the current invention because there was no consideration for symmetry.”

Applicant submits that the amended specification, in combination with statements already of record, makes clear that the invention provides methods for enhancing chemical structure diagram generation that were not known in the art prior to the filing date of the present application.

Rejection of Claims Under 35 U.S.C. § 103(a)

Claims 1, 5, and 9 are rejected under 35 U.S.C. § 103(a) as being obvious in view of Hu, et al., *Chemometrics and Intelligent Laboratory Systems*, 1/18/1999 (abstract) (“Hu”), or Shelley, et al., *J. Chem. Info. Comput. Sci.*, p. 247 (1979) (“Shelley”), in view of Fan et al., *J. Chem. Info. Comput. Sci.*, pp. 654-59 (1996) (“Fan”). Applicant respectfully disagrees. None of these references (either alone or in combination) teach “positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry,” as required by claims 1, 5, and 9. Accordingly, applicant submits that claims 1, 5, and 9 are nonobvious in view of the cited references.

The Hu abstract is concerned with the detection of topological symmetry, in a chemical structure, not the expression of such symmetry in a chemical structural diagram. Thus, Hu does not teach positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry. Specifically, Hu states, “an algorithm for detection of topological symmetry from a connection table is developed by the all-paths method” (emphasis added). The abstract also states that detection of symmetry is useful for searching for

a description of a molecular structure and for specifying the number of peaks in NMR spectra, in a structure evaluation process. Regarding structure generation, the abstract merely states that symmetry detection is useful for removing “irredundant connections”. This process is distinct from the process of the invention because it is concerned with harnessing symmetry to solve the problem of graphical isomorphism (determining if two connection tables are the same); it is not involved with depicting structures, i.e., SDG. To that end, Applicant notes that structure generation is distinct from structure *diagram* generation. Structure generation as described by Hu is limited to the creation of connection tables that indicate which atoms are bonded to each other. Structure diagram generation, in contrast, further includes, for example, assignment of coordinates that allows a picture (i.e., diagram) of the chemical structure to be generated by defining such properties as bond lengths and angles. For the foregoing reasons, Hu does not teach or suggest how to position symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry.

Shelley also does not teach positioning equivalent atoms and bonds in a chemical structure diagram in accordance with the identified symmetry. Shelley, like Hu, teaches an algorithm for detecting topological symmetry. In the first paragraph of the article, Shelley states that one problem the paper is concerned with is topological symmetry detection. Shelley goes on to state that a purpose of the article is to describe an approach to symmetry detection. Shelley, p. 247; *see also* p. 247, abstract (“Important principles in designing such algorithms [for topological symmetry perception] ... are presented.”). Shelley proceeds to provide step-wise explanations for various algorithms used to detect symmetry. Specifically, Shelley is concerned with identifying connection tables that are identical and removing redundant connection tables in an efficient fashion. As with Hu, however, Shelley is silent with respect to positioning

symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry.

The Office Action states that it would have been obvious to combine the teaching of Hu or Shelley regarding topological symmetry with Fan, which allegedly discloses detection of equivalent atoms from a connection table and displaying inherent equivalent atomic structures. Applicant disagrees. The amended claims do not require representing an instance of symmetry as a list of equivalent atoms and bonds. Thus, the Office Action's reasons for citing Fan are moot. Even so, Fan still does not teach or suggest positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry.

Accordingly, even assuming a motivation or suggestion to combine Hu or Shelley with Fan, the combined references still do not teach or suggest all of the claim limitations. To establish a prima facie case of obviousness, all claim limitations must be taught or suggested by the prior art. MPEP § 2143.03. As explained above, neither Hu nor Shelley teaches positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry. The combination of Fan with Hu or Shelley does not cure this deficiency. Fan, like Hu and Shelley, is concerned with the detection of equivalent atoms. Page 654, abstract ("A simple and efficient algorithm for the perception of constitutionally equivalent atoms in a target molecule is reported.") (emphasis added). Fan does not teach generation of chemical structure diagrams generally at all, let alone expressing chemical symmetry in a chemical structure diagram. Rather, Fan provides a new, more efficient, algorithm for detection of equivalent atoms. Page 654, col. 2 ("We therefore developed a new algorithm for the perception of constitutionally equivalent atoms from a connection table.... Our concern was the search for an efficient approach..."). The outcome of the method disclosed by Fan is shown in

Table 2 (p. 659), displaying vectors of equivalent sites for various exemplary chemical structures. Table 2 merely provides a list of equivalent vectors, thereby identifying instances of equivalency within a chemical structure. Fan does not cure the deficiencies of Hu and Shelley. Specifically, Fan does not teach or suggest positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry. Thus, none of the cited references teach all the elements of the claimed invention, either alone or in combination. Accordingly, Applicant submits that the claimed invention is nonobvious in view of Hu or Shelley further in view of Fan.

Claims 13-27 are rejected under 35 U.S.C. § 103(a) as being obvious in view of Hu or Shelley, in view of Fan et al., further in view of Chem3D Molecular Modeling and Analysis, User's_Guide CS Chem3D 4.0 for Windows and MacIntosh (1986-1997) ("Chem3D") and Razinger et al., *J. Chem. Inf. Comput. Sci.* 33:197-201 (1993) ("Razinger"). Applicant respectfully disagrees. Claims 13-27 depend from claim 1. As explained above, Hu or Shelley in combination with Fan do not teach or suggest positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry. Razinger and Chem3D do not cure this deficiency. Razinger, like Hu, Shelley and Fan merely discloses algorithms for the detection of symmetry. Indeed, in its abstract, Razinger states that several algorithms, including the algorithm of Shelley, are compared. Thus, Razinger provides no further teaching regarding expressing symmetry in a chemical structural diagram. Chem3D, in addition to not teaching or suggesting positioning symmetrically equivalent atoms and bonds in a chemical structure diagram in accordance with an identified symmetry, also did not assess symmetry. Moreover, The Office Action states that Chem3D discloses symmetry operations and properties and their manipulations in molecular modeling and analysis. Applicant has reviewed

chapters 4 and 5 of the Chem3D User's Guide referenced above and has failed to find references to symmetry operations as described in the Office Action. If this reference continues to be cited, Applicant requests clarification of the identity of the reference and a more detailed description of the pertinent subject matter. For the reasons stated above, the combination of Razinger and Chem3D does not provide the required teaching to cure the defects in the other references. Accordingly, Applicant submits that claims 13-27 are nonobvious.

Conclusion

In view of the foregoing remarks, Applicants submit that all pending claims are in condition for allowance, which action is earnestly solicited.

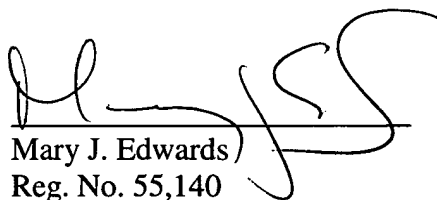
Applicants respectfully request an early and favorable reconsideration and issuance of this application as amended herein. The Examiner is encouraged to contact the undersigned to expedite prosecution of this application.

Applicants also include a petition for a one-month extension of time to extend the period for response up to and including May 24, 2006. An authorization to charge the associated small entity fee of \$60.00 to our Deposit Account No. 08-0219 accompanies this response.

No other fees are believed to be due in connection with this submission. However, if any fees are due in connection with this application, please charge them to our Deposit Account No. 08-0219.

Respectfully submitted,

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